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6-AMINOPIRIDIN-2-KARBON KISLOTASINING $[CU(L)_2(H_2O)_2]$ VA $[ZN(L)_2(H_2O)_2]$ TARKIBLI KOMPLEKS BIRIKMALARINI OLISH VA ULARNING TADQIQI

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Annotation: Ushbu maqolada Cu(II) va Zn(II) ionlarining 6-aminopiridin-2-karbon kislota bilan kompleks birikmalarini olish jarayoni, eritma muhiti, kompleks birikmaning tuzilishini aniqlashda rentgen tuzilishi tahlili, uning molekulyar va kristall tuzilishi yoritilgan.

Keywords: 3d- metallari, kompleks birikmalar, 6-aminopiridin-2-karbon kislota kislotasi, kimyoviy xususiyatlar.

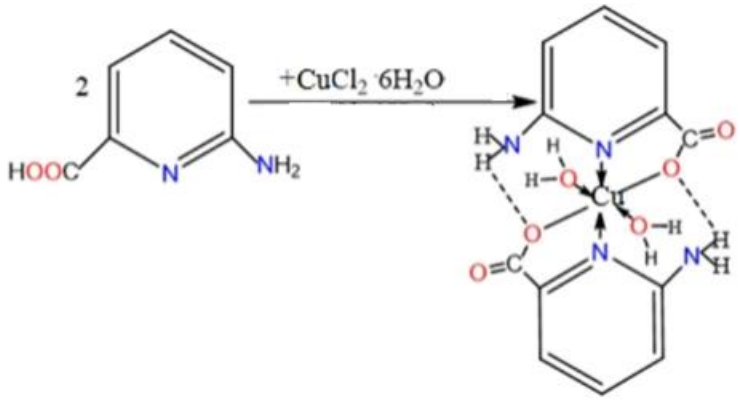
Kirish. Hozirgi kunda kompleks birikmalar kimyosi zamonaviy kimyo fanining eng tez rivojlanayotgan yo‘nalishlaridan biri hisoblanadi. Ayniqsa, o‘tish metallari, jumladan Cu(II) va Zn(II) ionlarining turli xil organik ligandlar bilan hosil qilgan kompleks birikmalarini o‘rganish ilmiy va amaliy jihatdan katta ahamiyat kasb etmoqda. Bunday komplekslar biologik faolligi, katalitik xossalari hamda sanoat va tibbiyotdagi qo‘llanilish imkoniyatlari bilan ajralib turadi.

Azot va kislorod donor atomlariga ega bo‘lgan organik ligandlar, xususan, piridin hosilalari koordinatsion birikmalar hosil qilishda muhim rol o‘ynaydi [1]. Shunday ligandlardan biri bo‘lgan 6-aminopiridin-2-karbon kislota o‘z tarkibida bir vaqtning o‘zida amin guruhi ($-NH_2$), piridin halqasi va karboksil guruhi (-COOH) ni saqlaganligi sababli ko‘p markazli koordinatsiya qobiliyatiga ega. Bu esa uning metall ionlari bilan turli xil barqaror kompleks birikmalar hosil qilishiga imkon beradi.

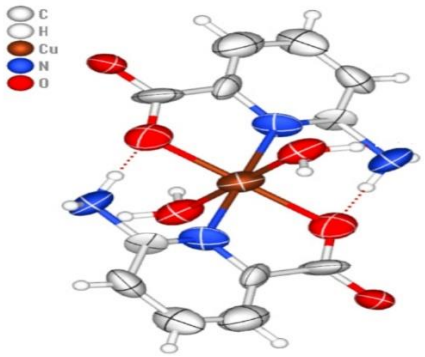
Ushbu ligandlarning kompleks birikmalarni o‘rganish muhim ahamiyat kasb etadi. Ular biologik faol bo‘lganligi uchun keng qo‘llaniladi. Ayniqsa bu borada 3d-metall komplekslari dori ta’sirini samarali ortirishda muhim rol o‘ynaydi [2]. Metall ionining tabiati, shuningdek ligand turi tufayli farmako logik faoliyatda muhim ahamiyatga ega muhim ahamiyatga ega turli metallar va ligandlar har xil biologik xususiyatga ega [3]. Jumladan karboksilat guruhi tutgan ligand (piridindikarbon, aminopiridinkarbon kislota, glutamat, aspartat,) va tufayli qiziqarli soha bo‘lib kelgan. Ikki yoki undan ortiq karboksilik guruhlarning turli burchaklardagi bog‘lanishi 1D (uzun zanjir), 2D (varaq) yoki 3D (qafas) tuzilishini shakllantirishga imkon beradi [4,5].

Kompleks birikma sintezi.

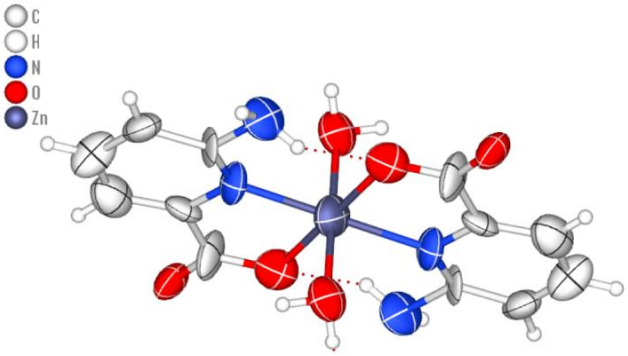
Mis(II)xlorid kristallogidratidan $CuCl_2 \cdot 6H_2O$ 0.1185 gr (0.5 mmol), 0.138 gr Eritmalar aralashtirildi. So‘ngra magnitli aralashtirgich yordamida 60 ^{0}C da 30 minut davomida intensiv aralashtirildi. Eritma xona haroratida qoldirildi. Natijada 10 kundan so‘ng idish tubida och yashil rangli kompleks birikma kristali o‘sganligi kuzatildi. RTT analizi uchun yaroqli kristallar ajratilib, tekshirilganda $[Cu(L)_2(H_2O)_2]$ tarkibli ekanligi aniqlandi. Unumi 86 %. $[Zn(L)_2(H_2O)_2]$ kompleksi ham ushbu usulda olingan.



1-sxema. $[Cu\ (L)_2\ (H_2O)_2]$ kompleksining molekulyar tuzilishi



2-rasm.$[Cu\ (L)_2\ (H_2O)_2]$ kompleksining molekulyar tuzilishi



3-rasm.$[Zn(L)_2\ (H_2O)_2]$ kompleksining molekulyar tuzilishi

$[Cu(L)_2\ (H_2O)_2]$ kompleksining singoniyasi triclinic bo‘lib, a, b, c ° mos ravishda 110.66(2), 97.945(19), 104.949(15). Markaziy atom Cu(II) ning koordinatsion soni 6, sp^3d^2 holatda gibridlanishga ega. Ushbu kompleks birikmada ikkala APY anioni Cu(II) ioniga karboksil ionidagi kislorod atomi va piridin halqasidagi azot atomi orqali bidentant holatda koordinatsiyalangan. Bundan tashqari ikki suv molekulasi ham markaziy atomga donor-akseptor bog‘lanish orqali bog‘langan, natijada oktaedrik shakl yuzaga kelgan. Cu1-O1 bog‘lanish uzunligi 2.029(4) Å, Cu1-O3 bog‘lanish uzunligi 2.121(5)Å, Cu1-N1 2.096(5) Å, Ni1-O1_a 2.029(4) Cu1-O3_a 2.121(5)

hamda Cu 1-N1_a 2.096(5) Å. Tashqi sferada bir molekula sirka kislotasi va suv molekulasi o‘zaro vodorod bog‘lanish orqali bog‘langan. Kompleksning ichki sferada N2--H2B..O1 vodorod bog‘lanishi mavjud.

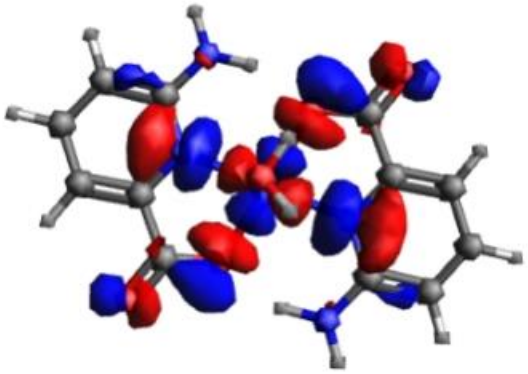
Olingan kompleks birikmalarning kvant -kimyoviy hisoblash natijalari

$[Cu(L)_2(H_2O)_2]$ va $[Zn(L)_2(H_2O)_2]$ komplekslari B3LYP-D4/ def2-TZVP usullarida energetik ko‘rsatgichlari hisoblandi

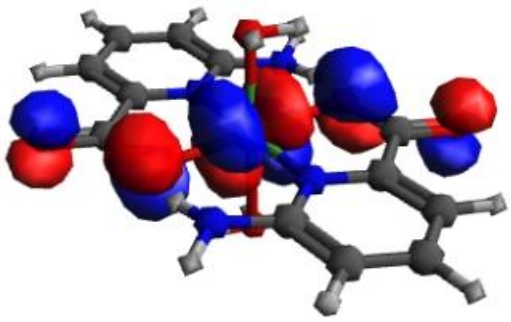
1-jadval.

B3LYP-D4/def2-TZVP tomonidan uchlik holatdagi Cu va Zn kompleksining MO energiyalari va energiya bo‘shlig'i (DE)

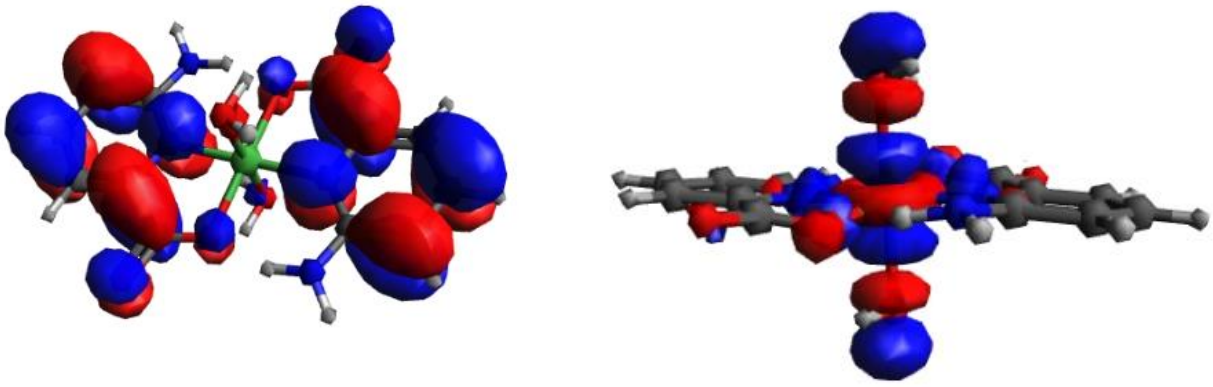
	B3LYP-D4/def2-TZVP					
	HOMO (α)	HOMO(β)	LUMO (α)	LUMO (β)	ΔE(α)	ΔE(β)
$[Cu(L)_2(H_2O)_2]$	-4.61	-5.26	-2.53	-3.47	2.08	1.79
Keltirilgan MO-larda p va d ulushi (%):	p: 52.15 d:42.54	p: 19.50 d: 79.77	p: 91.37 d: 7.18	p: 15.47 d: 79.09		
	B3LYP-D4/ def2-TZVP					
$[Zn(L)_2(H_2O)_2]$	HOMO (α)	HOMO(β)	LUMO (α)	LUMO (β)	ΔE(α)	ΔE(β)
	-6.16	-6.24	-1.64	-1.63	4.52	4.61
Keltirilgan MO-larda p va d ulushi (%):	p: 75.67 d: 19.61	p: 93.96 d: 5.42	p: 90.93 d: 7.38	p: 90.88 d: 7.40		



HOMO (α) Cu

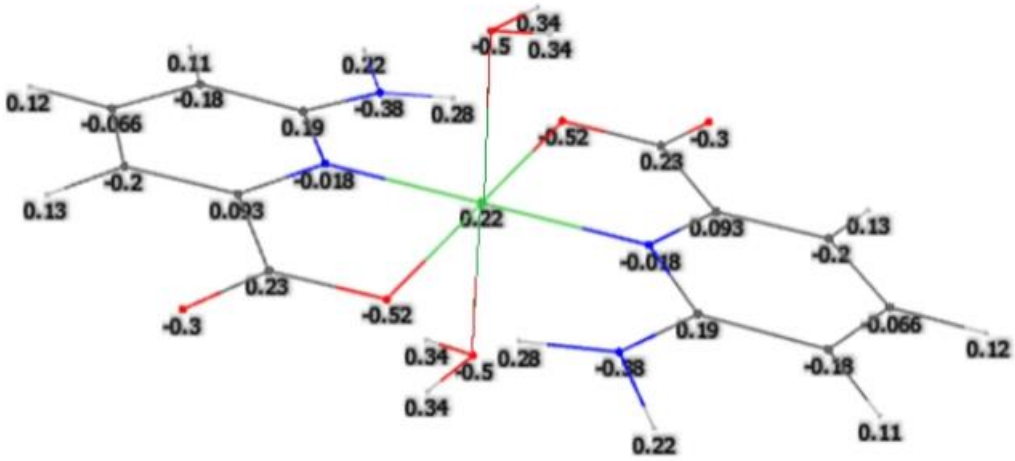


HOMO(β) Cu

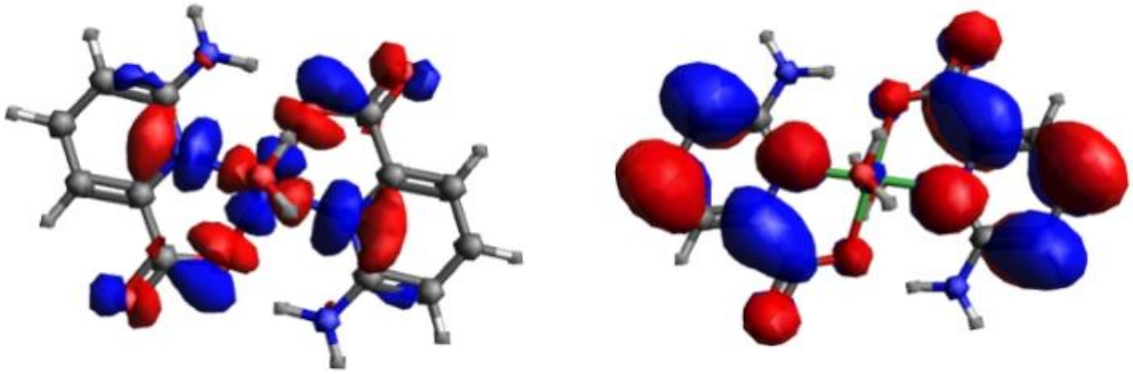


LUMO (α) Cu LUMO (β) Cu

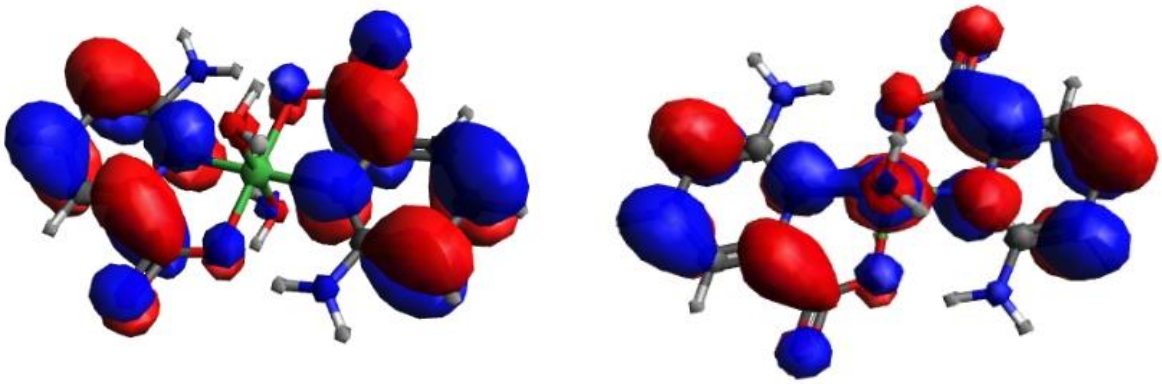
4-rasm. $[Cu(L)_2(H_2O)_2]$ kompleksining HOMO va LUMO si



5-rasm. Cu kompleksining B3LYP-D4/def2-TZVP tomonidan atom zaryadining taqsimlanishi

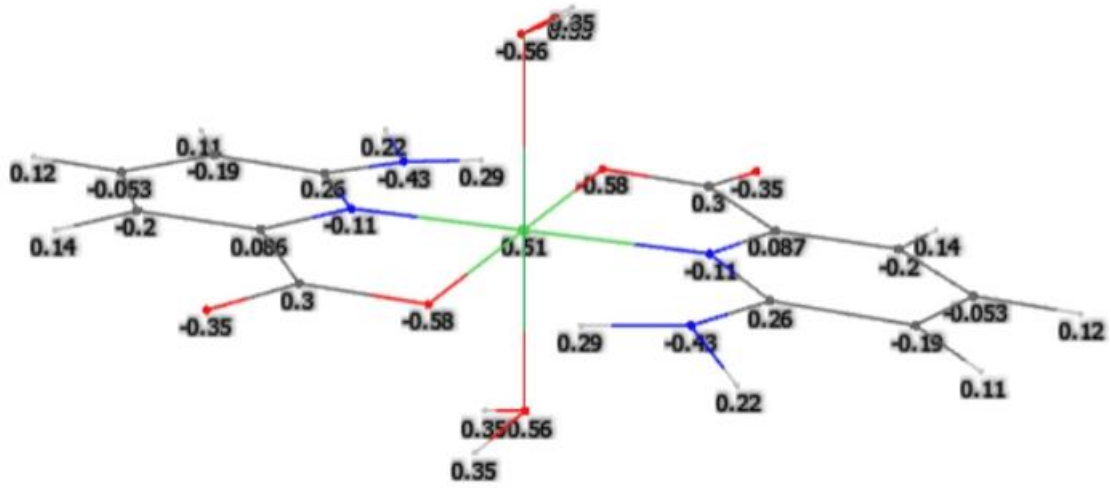


HOMO (α) Zn HOMO(β) Zn

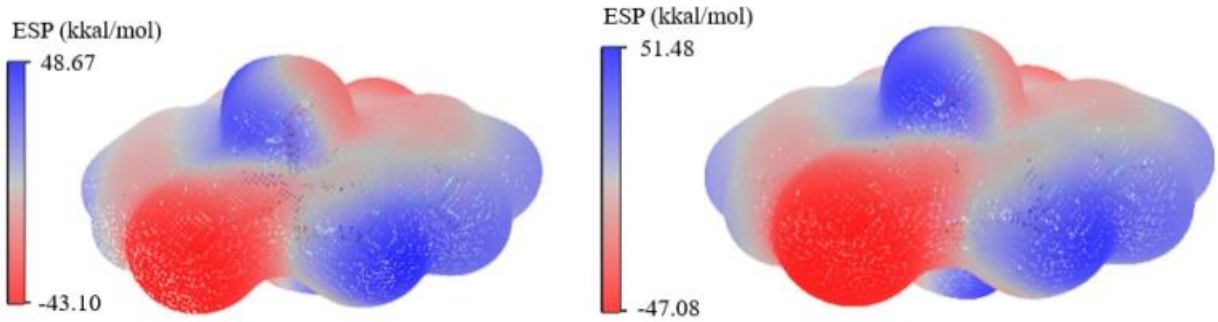


LUMO (α) Zn LUMO (β) Zn

6-rasm. $[Zn(L)_2(H_2O)_2]$ kompleksining HOMO va LUMO si



7-rasm. Zn kompleksining B3LYP-D4/def2-TZVP tomonidan atom zaryadining taqsimlanishi



8-rasm. Cu (chapda) va Zn (o‘ngda)kompleksining ESP sathi maksimum va minimumlari (B3LYP usuli)

$[Cu(L)_2(H_2O)_2]$ va $[Zn(L)_2(H_2O)_2]$ komplekslarining ESP tahlili B3LYP-D4/ def2-TZVP usulida tahlil qilindi. Eng katta maksimum har ikki kompleksdagi ligand

halqasining H atomlari yaqinida joylashgan (mos ravishda 48.67 kkal/mol va 51.48 kkal/mol energiya qiymatlariga ega). Eng past minimum kompleksning –COO guruhining O atomlari yaqinida joylashgan (mos ravishda -43.10 kkal/mol va -47.08 kkal/ mol).

Xulosa. Cu(II) va Zn(II) ionlarining 6-aminopiridin-2-karbon kislota bilan kompleks birikmalari olinib, monokristali o‘stirildi. Ularning tuzilishi RTT (rentgen tuzilishi tahlili) yordamida aniqlandi. Izostrukturali kompleks birikmalarda markaziy atomning koordinatsion soni 6, sp^3d^2 holatda gibridlanishga ega. 6-aminopiridin-2-karbon kislota ligandi markaziy atomga bidentant holatda koordinatsiyalangan. Olingan kompleks birikmalarning energetik ko‘rsatgichlari B3LYP-D4/ def2-TZVP usullarida hisoblandi.

Foydalanilgan adabiyotlar ro‘yxati.

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